





1 SBMLToolkit.jl: A Julia package for generating 2 ModelingToolkit models from SBML

3 Paul F. Lang ^{1,2} , Anand Jain¹, and Chris Rackauckas ^{1,3}

4 ¹ JuliaHub, USA ² Department of Biochemistry, University of Oxford, UK ³ Computer Science and
5 Artificial Intelligence Laboratory (CSAIL), Massachusetts Institute of Technology, USA  Corresponding
6 author

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

Editor: [Open Journals](#) 

Reviewers:

- [@openjournals](#)

Submitted: 01 January 1970

Published: unpublished

License

Authors of papers retain copyright
and release the work under a
Creative Commons Attribution 4.0
International License ([CC BY 4.0](#)).

7 Summary

8 SBMLToolkit.jl is a lightweight tool to import models specified in the Systems Biology Markup
9 Language (SBML) ([Hucka et al., 2003](#)) into the Julia SciML ecosystem. SBMLToolkit uses
10 the SBML.jl ([Kratochvíl & Giordano, 2021](#)) wrapper of the libSBML library ([Bornstein et al.,
11 2008](#)) to lower dynamical SBML models into dynamical systems.

12 Statement of need

13 Julia is a general purpose programming language that was designed for simplifying and ac-
14 celerating numerical analysis and computational science. Building on the computer algebra
15 system Symbolics.jl ([Gowda et al., 2022](#)), many high-performing solvers for differential equa-
16 tions have been developed in Julia ([Rackauckas & Nie, 2017](#)). In particular the Scientific
17 Machine Learning (SciML) ecosystem of Julia packages includes ModelingToolkit.jl ([Ma et al.,
18 2021](#)), a modeling framework for high-performance symbolic-numeric computation in scientific
19 computing and scientific machine learning. It allows for users to give a high-level description
20 of a model for symbolic preprocessing to analyze and enhance the model. ModelingToolkit
21 can automatically generate fast functions for model components, along with automatically
22 sparsifying and parallelizing the computations. This enabled highly performing solvers of
23 differential equations, parameter optimisation algorithms and methodologies for automated
24 model discovery ([Rackauckas et al., 2020](#)). To give the systems biology community easy access
25 to SciML, we developed SBMLToolkit.jl, an importer for SBML models. Together with the
26 development of other tools such as CellMLToolkit.jl ([Irvanian et al., 2021](#)) for import of
27 CellML models ([Cuellar et al., 2003](#)), Catalyst.jl ([Loman et al., 2022](#)) for de-novo specification
28 of ModelingToolkit models, and COBREXA.jl ([Kratochvíl et al., 2021](#)) for constraint-based
29 modelling, we hope that SBMLtoolkit.jl will help to catalyse the development of further
30 Julia tools in the bioscience domain to ultimately accelerate research on biological systems
31 ([Figure 1](#)).

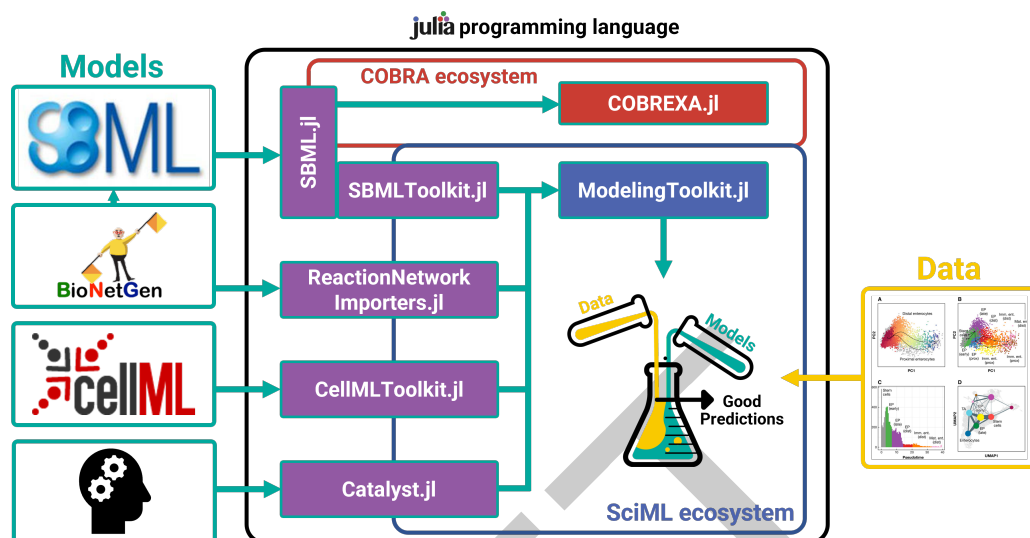


Figure 1: The Julia ecosystem for systems biology. SBMLToolkit.jl links SBML and BioNetGen (Blinov et al., 2004; Harris et al., 2016) models to the SciML ecosystem.

Acknowledgements

We would like to thank Miroslav Kratochvil and Samuel Isaacson for supporting the development efforts. PFL acknowledges funding from the Engineering and Physical Sciences Research Council [grant number EP/L016494/1].

References

- Blinov, M. L., Faeder, J. R., Goldstein, B., & Hlavacek, W. S. (2004). BioNetGen: Software for rule-based modeling of signal transduction based on the interactions of molecular domains. *Bioinformatics*, 20(17), 3289–3291. <https://doi.org/10.1093/bioinformatics/bth378>
- Bornstein, B. J., Keating, S. M., Jouraku, A., & Hucka, M. (2008). LibSBML: An API library for SBML. *Bioinformatics*, 24(6), 880–881. <https://doi.org/10.1093/bioinformatics/btn051>
- Cuellar, A. A., Lloyd, C. M., Nielsen, P. F., Bullivant, D. P., Nickerson, D. P., & Hunter, P. J. (2003). An Overview of CellML 1.1, a Biological Model Description Language. *SIMULATION*, 79(12), 740–747. <https://doi.org/10.1177/0037549703040939>
- Gowda, S., Ma, Y., Cheli, A., Gwóźdz, M., Shah, V. B., Edelman, A., & Rackauckas, C. (2022). High-performance symbolic-numeric via multiple dispatch. *ACM Commun. Comput. Algebra*, 55(3), 92–96. <https://doi.org/10.1145/3511528.3511535>
- Harris, L. A., Hogg, J. S., Tapia, J.-J., Sekar, J. A. P., Gupta, S., Korsunsky, I., Arora, A., Barua, D., Sheehan, R. P., & Faeder, J. R. (2016). BioNetGen 2.2: Advances in rule-based modeling. *Bioinformatics*, 32(21), 3366–3368. <https://doi.org/10.1093/bioinformatics/btw469>
- Hucka, M., Finney, A., Sauro, H. M., Bolouri, H., Doyle, J. C., Kitano, H., Arkin, A. P., Bornstein, B. J., Bray, D., Cornish-Bowden, A., Cuellar, A. A., Dronov, S., Gilles, E. D., Ginkel, M., Gor, V., Goryanin, I. I., Hedley, W. J., Hodgman, T. C., Hofmeyr, J.-H., ... SBML Forum. (2003). The systems biology markup language (SBML): A medium for representation and exchange of biochemical network models. *Bioinformatics (Oxford, England)*, 19(4), 524–531. <https://doi.org/10.1093/bioinformatics/btg015>

- 58 Iravanian, S., Rackauckas, C., & Jain, A. (2021). CellMLToolkit.jl. In *GitHub repository*.
59 GitHub. <https://github.com/SciML/CellMLToolkit.jl>
- 60 Kratochvíl, M., & Giordano, M. (2021). SBML.jl. In *GitHub repository*. GitHub. <https://github.com/LCSB-BioCore/SBML.jl>
- 62 Kratochvíl, M., Heirendt, L., Wilken, S. E., Pusa, T., Arreckx, S., Noronha, A., Aalst,
63 M. van, Satagopam, V. P., Ebenhöf, O., Schneider, R., Trefois, C., & Gu, W. (2021).
64 COBREXA.jl: constraint-based reconstruction and exascale analysis. *Bioinformatics*, 38(4).
65 <https://doi.org/10.1093/bioinformatics/btab782>
- 66 Loman, T., Ma, Y., Ilin, V., Gowda, S., Korsbo, N., Yewale, N., Rackauckas, C. V., &
67 Isaacson, S. A. (2022). Catalyst: Fast biochemical modeling with julia. *bioRxiv*. <https://doi.org/10.1101/2022.07.30.502135>
- 69 Ma, Y., Gowda, S., Anantharaman, R., Laughman, C., Shah, V., & Rackauckas, C. (2021).
70 *ModelingToolkit: A composable graph transformation system for equation-based modeling*.
71 <https://arxiv.org/abs/2103.05244>
- 72 Rackauckas, C., Ma, Y., Martensen, J., Warner, C., Zubov, K., Supekar, R., Skinner, D., &
73 Ramadhan, A. (2020). Universal Differential Equations for Scientific Machine Learning.
74 *arXiv:2001.04385 [Cs, Math, q-Bio, Stat]*. <http://arxiv.org/abs/2001.04385>
- 75 Rackauckas, C., & Nie, Q. (2017). DifferentialEquations.jl – a performant and feature-rich
76 ecosystem for solving differential equations in julia. *The Journal of Open Research Software*,
77 5(1). <https://doi.org/10.5334/jors.151>

DRAFT